Workshop #4: Best Practices of the Quantum-Mechanics (QM) driven Macromolecular Refinement

Date/Time	Friday, July 7, 2023 @ 8:50 AM ET			Registration Fees
Location	Falkland			Regular: $120 Per Person Retired: $120 Per Person PostDoc: $120 Per Person Student: $120 Per Person
Max Capacity	50			
Main Contact	Lance M. Westerhoff			

Description

Typically, macromolecular refinement procedures utilize simplistic restraints on bond lengths, angles and so on to ensure the reasonable geometry of the model after the refinement. A significant drawback of using conventional stereochemical-restraints is the lack of the chemical reality observed in the refined model as such intra-molecular restraints, no matter how accurate, do not account for critical atomic, inter-molecular interactions such as hydrogen bonds, dispersion, electrostatics, polarization, and charge transfer. Furthermore, for each ligand in the structure requires a custom description of the geometry details in the form of Crystallographic Information File (CIF). Unfortunately, creation of accurate CIF's is often a nontrivial and error-prone task. One way to overcome those problems and improve the X-ray structure quality is to incorporate a quantum mechanics (QM) description of the model into the refinement procedure. Recent advances in the field (Borbulevych et al, Acta Cryst. 2018, D74,1073) have allowed us to routinely perform QM and mixed-QM/MM-driven refinement on any size protein-ligand system. This level of refinement consistently leads to models with significantly improved ligand and protein:ligand bonded and non-bonded inter- and intra-molecular geometries, improved hydrogen bonding networks (including with bridging waters), more accurate tautomer/protomer and rotomer states, and overall improved fit to density. Despite obvious benefits of QM and QM/MM refinement, the use of such advanced techniques is still relatively rare in the crystallographic community. The proposed workshop fits the purpose to educate crystallographers on the theory, benefits, and practical details of conducting the QM driven protein refinement. Detailed tutorials planned for this workshop aim to lower the barrier for the crystallographic community to use the available QM tools (both locally and in the cloud) in routine refinement of any macromolecular structures.

Schedule*

Time	Instructor/Topic
8:50 AM - 9:00 AM ET	Introduction
9:00 AM - 9:45 AM ET	Overview of the QM driven macromolecular Refinement (lecture)
9:45 AM - 10:00 AM ET	Coffee Break
10:00 AM - 11:00 AM ET	XModeScore - a versatile tool to distinguish protomers, tautomers and flip states (lecture)
11:00 AM - 12:00 PM ET	Impact of QM refinement on the binding affinity prediction in SBDD (lecture)
12:00 PM - 1:30 PM ET	Lunch (included)
1:30 PM - 3:30 PM ET	Common techniques of running QM Refinement - Tutorials
3:30 PM - 3:50 PM ET	Coffee Break
3:50 PM - 4:50 PM ET	XModeScore Tutorials
4:50 PM - 5:00 PM ET	Final Remarks

Tentative and subject to change.

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